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# A new four-parameter potential function for stable diatomic molecules

M Rafi*, A Bakry, N Al-Senany and Fayyazuddin**
Department of Physics, King Abdul Aziz University, P O Box 9028, Jeddah 21413 Saudi Arabia
**Department of Physics, Quaid-i-Azam University, Islamabad
E-mail : professor rafi@yahoo com

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**Abstract** : A new four-parameter empirical potential function has been proposed for the stable states of diatomic molecules The parameters of the function are obtained in terms of known experimental values of the spectroscopic constants A comparative study of the potential curves of the proposed function with those of six other functions and the Rydberg-Klein-Rees data, has been made for 15 molecules

**Keywords** Empirical model, potential function, diatomic molecule

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There are different methods for the calculation of potential curves for molecules. Quantum mechanical methods are found cumbersome for heavy molecules due to mathematical and computational difficulties. The Rydberg-Klein-Rees (RKR) [1–3] method is regarded as a reliable method for obtaining the potential curves This method is suitable when sufficient spectroscopic data are available. The third method is to find out an analytical form to represent the potential function. The parameters of this function are related to the spectroscopic constants : the bond length $r_e$, the force constant $k_e$, the vibrational-rotational coupling constants $\alpha_e$, the anharmonicity constant $\omega_e x_e$ and the dissociation energy $D_e$. A number of 3 to 5 parameter functions are found in literature [4–16]. A single function is not adequate for all the molecules and therefore new functions are proposed now and then. We propose a four-parameter double exponential function which is a modification of the Morse function as given below :

$$V(x) = D_e\left[1 - e^{-ax}\right]^2\left[1 + c\tanh x\right], \tag{1}$$

where $x = r - r_e$, $r$ being the internuclear distance, $c$ and $a$ are the parameters to be determined in terms of spectroscopic constants.

A potential function of stable electronic states of diatomic molecules obeys the following conditions as given by Varshni [8] .

$$V_\infty - V(r_e) = D_e \tag{2}$$

$$\left.\frac{dV}{dr}\right|_{r=r_e} = 0, \tag{3}$$

$$\left.\frac{d^2V}{dr^2}\right|_{r=r_e} = k_e, \tag{4}$$

$$\left.\frac{d^3V}{dr^3}\right|_{r=r_e} = Xk_e, \tag{5}$$

where $X$ is termed the cubic force constant Eq. (1) can also be written in the following form

$$V(x) = D_e\left[1 - e^{-ax}\right]^2\left[1 + c\frac{e^{ax} - e^{-ax}}{e^{ax} + e^{-ax}}\right]. \tag{6}$$

We apply the conditions given in eqs (2–5) to eq. (6) and obtain

$$V(x)|_{x=0} = 0, \tag{7}$$

$$\left.\frac{dV(x)}{dx}\right|_{x=0} = 0, \tag{8}$$

$$\left.\frac{d^2V(x)}{dx^2}\right|_{x=0} = 2D_e a^2, \tag{9}$$

$$\left.\frac{d^3V(x)}{dx^3}\right|_{x=0} = -6D_e a^3(1-c). \tag{10}$$

Eqs. (4) and (9) give , $2D_e a^2 = k_e$,

$$ar_e = \sqrt{\frac{k_e r_e^2}{2D_e}} = \Delta^{\frac{1}{2}}, \tag{11}$$

$$\text{where } \Delta = \frac{k_e r_e^2}{2D_e}. \tag{12}$$



*Author for correspondence

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